

The jamming transition of Granular Media

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Abstract

A statistical mechanical approach to granular material is proposed. Using lattice models from standard Statistical Mechanics and results from a mean field replica approach we find a jamming transition in granular media closely related to the glass transition in super-cooled liquids. These models reproduce the logarithmic relaxation in granular compaction and reversible-irreversible lines, in agreement with experimental data. The models also exhibit aging effects and breakdown of the usual fluctuation dissipation relation. It is shown that the glass transition may be responsible for the logarithmic relaxation and may be related to the cooperative effects underlying many phenomena of granular materials such as the Reynolds transition.

I. INTRODUCTION

Despite their importance for industrial applications, non-thermal disordered systems as granular media have just recently begun to be systematically studied in the physics community [1]. In particular, concepts from Statistical Mechanics seems to be successful to describe these systems as suggested in his pioneering work by Edwards [2]. Actually, granular

media are composed by a large number of single grains and, as much as systems of standard Statistical Mechanics, each of their macroscopic states corresponds to a huge number of microstates. Furthermore, they show very general reproducible macroscopic behaviours whose general properties are not material specific and which are statistically characterised by very few control parameters, such as their density, load or amplitude of external drive [1]. Granular media are “non-thermal” systems since thermal energy plays no role with respect, for instance, to gravitational energies involved in grain displacements, however, thermal motion can be replaced by agitation induced by shaking or other driving and this allows the system to explore its space of configurations.

A “tapping” dynamics has several control parameters. A very important one, related to the amplitude of vibrations of the external driving, has appeared to be the adimensional ratio $\Gamma_{ex} = a/g$ [1,3], where a is the shake peak acceleration and g the gravity acceleration constant. It has been suggested that Γ_{ex} plays a role very similar to “temperature” in thermal systems. For simplicity, below we suppose the characteristic frequency, ω , of external driving is fixed, and actually in typical experiments as those in Ref.s [3,4] we are interested in, it plays a minor role with respect to Γ_{ex} (see [1]). Material parameters such as restitution, friction coefficients, presence of moisture, etc., are also to be usually considered, but they generally do not affect the overall behaviours.

Experimentally it is found that at low Γ_{ex} relaxation processes as density compaction under tapping are logarithmically slow. An essential ingredient in the dynamics of dense granular media is, instead, the presence of “frustrating” mechanisms on the motion of grains due to steric hindrance and hard core repulsion. We have introduced Frustrated Lattice Gases to describe the dynamics of granular materials in the regime of high densities or not too strong shaking [5–7]. They interestingly allow to interpret, in a single framework, several different properties of granular media ranging from logarithmic compaction, density fluctuations, “irreversible-reversible” cycles, aging, breakdown of fluctuation dissipation relation, segregation, to avalanches effects, the Reynolds transition and several others [6,7,13,14,25]. In particular they predict the existence of a definite “jamming” transition in granular media,

in strict correspondence with the glass transition of glass formers and spin glasses [1,8–10]. Furthermore, they are new important applications of the statistical mechanics to powders [2,11].

II. FRUSTRATED LATTICE GAS MODELS FOR GRANULAR MEDIA

The very simple schematic models for gently shaken granular media we introduced are based on a drastic reduction of the degrees of freedom of the systems to those we suppose are essential. The models consist of a system of elongated grains which move on a lattice. Grains are subject to gravity and, eventually, to shaking, which is simulated with a driven diffusion like Monte Carlo dynamics. The crucial ingredient of the models is the presence of geometric constraints on the motion of the grains, thus, they have been called Frustrated Lattice Gases [5,6]. Particles in our models occupy the sites of, say, a square (or cubic) lattice (see Fig.1). They have also an internal degree of freedom $S_i = \pm 1$ corresponding to their possible “orientations” along the two lattice axes. Two nearest neighbour sites can be both occupied only if the particles do not overlap.

Each “experimental” tap can be divided in two parts: one where the grains average kinetic energy is finite and a second where it goes to zero. Thus, in our models grains undergo a schematic driven diffusive Monte Carlo (MC) dynamics: in absence of vibrations they are subject only to gravity and they can move just downwards always fulfilling the non overlap condition; the presence of vibration is introduced by allowing the particles to diffuse with a probability p_{up} to move upwards and a probability $p_{down} = 1 - p_{up}$ to move downwards. The quantity $-\ln(x_0)/2$, with $x_0 = p_{up}/p_{down}$, as we will see, plays the role of an effective temperature and can be related to the experimental tap vibrations intensity, Γ_{ex} .

A. Hamiltonian description

The general model introduced above can be described in terms of a standard lattice gas of Statistical Mechanics [5,6]. The system Hamiltonian must have an hard core repulsion term ($J \rightarrow \infty$):

$$H_{HC} = J \sum_{\langle ij \rangle} f_{ij}(S_i, S_j) n_i n_j . \quad (1)$$

Here $n_i = 0, 1$ are occupancy variables describing the positions of grains, $S_i = \pm 1$ are “spin” variables associated to the orientations of the particles, J represents the infinite repulsion felt by the particles when they have the wrong orientations. The hard core repulsion function $f_{ij}(S_i, S_j)$ is 0 or 1 depending whether the configuration S_i, S_j is right (allowed) or wrong (not allowed), see Fig.1.

The choice of $f_{ij}(S_i, S_j)$ depends on the particular model. In particular, here we consider two models: the Tetris and the Ising Frustrated Lattice Gas (IFLG). The Tetris model is made of elongated particles (see Fig. 1), which may point in two (orthogonal) directions coinciding with the two lattice bond orientations. In this case $f_{ij}(S_i, S_j)$ is given by [7] $f_{ij}^{Tetris}(S_i, S_j) = 1/2(S_i S_j - \epsilon_{ij}(S_i + S_j) + 1)$ here $\epsilon_{ij} = +1$ for bonds along one direction of the lattice and $\epsilon_{ij} = -1$ for bonds on the other. In order to have a non trivial behaviour the dynamics of the Tetris has a crucial *purely kinetic constraint*: particles can flip their “spin” only if three of their own neighbours are empty.

A real granular system may contain more disorder due to the presence of a wider grain shape distribution or to the absence of a regular underlying lattice. Typically, each grain moves in the disordered environment generated by its neighbours. In order to schematically consider these effects within the above context, an other kind of “frustrated lattice gas” was introduced, made of grains moving in a lattice with quenched geometric disorder. Such a model, the Ising Frustrated Lattice Gas (IFLG), has the following hard core repulsion function, $f_{ij}(S_i, S_j)$ [6]: $f_{ij}^{IFLG}(S_i, S_j) = 1/2(\epsilon_{ij} S_i S_j - 1)$ where $\epsilon_{ij} = \pm 1$ are quenched random interactions associated to the edges of the lattice, describing the fact that particles must sat-

isfy the geometric constraint of the environment considered as “practically” quenched (see Fig.1). The IFLG shows a non trivial dynamics *without* the necessity to introduce kinetic constraints.

The phase diagram of the Tetris Hamiltonian corresponds to the usual antiferromagnetic Ising model with dilution. The Hamiltonian of the IFLG exhibits richer behaviours. In the limit where all sites are occupied ($n_i = 1 \forall i$), it becomes equal to the usual $\pm J$ Ising Edwards-Anderson Spin Glass [10]. In the limit $J \rightarrow \infty$ (which we consider below), a version of Site Frustrated Percolation is recovered [15,16].

The other important contribution to the full Hamiltonian of a granular pack we consider below must be gravitational energy: $\mathcal{H} = H_{HC} + H_G$, where $H_G = g \sum_i n_i y_i$, and g is the gravity constant and y_i is the height of particle i (grains mass and lattice spacing are set to unity). The temperature, T , of the present Hamiltonian system (with $J = \infty$) is related to the ratio $x_0 = p_{up}/p_{down}$ via the following relation: $e^{-2g/T} = x_0$. It is useful to define the adimensional quantity $\Gamma \equiv 1/\ln(x_0^{-1/2}) = T/g$, which we assume plays the same role as the amplitude of the vibrations in real granular matter, that is Γ is a smooth function of Γ_{ex} .

It is easy to show [25] that if the system reaches equilibrium, the temperature T is:

$$T^{-1} = \frac{\partial \ln \Omega}{\partial E} \quad (2)$$

where Ω is the number of configurations corresponding to the gravitational energy E . Note that for samples with constant particle density, E is proportional to the volume and thus $1/T$ coincides with Edwards’ compactivity [2] apart from a proportionality constant.

III. THE DYNAMICS OF COMPACTION

To describe experimental observations about grain density relaxation under a sequence of taps a logarithmic law was proposed in Ref. [3]:

$$\rho(t_n) = \rho_\infty - \Delta\rho_\infty/[1 + B \ln(t_n/\tau_1 + 1)] \quad (3)$$

This law has proved to be satisfied very well by relaxation data in the IFLG model [6], which can be excellently rescaled with experimental data. In Fig.2 MC compaction data for four different amplitudes, Γ , as well as the experimental data for three different amplitudes, Γ_{ex} , are collapsed on a single curve using eq.(3). The agreement is very satisfactory (details about these data are in Ref. [6]).

Interestingly, the results from Tetris are similar [7], but the asymptotic density ρ_∞ is numerically indistinguishable from 1, thus almost independent on x_0 , a fact in contrast with both IFLG and experimental results [3].

IV. GLASSY BEHAVIOURS OF GRANULAR MEDIA

We have seen that compaction shows extremely long relaxation times. Actually we show that granular systems are typically in off equilibrium configurations and that they may undergo a “jamming” transition. In particular, in the same framework of the above models, we show how experimental results about “memory” effects (the so called “irreversible-reversible” cycles) outline the existence of a dynamical glassy transition, which can be defined in a similar way to the glassy transition in real glass formers.

It has been shown in mean field approximation [17] and numerically for finite dimensional systems [16], that the IFLG, in absence of gravity, exhibits a spin glass (SG) transition at high density (or low temperature) similar to the one found in the p-spin model. J.J. Arenzon has extended the mean field solution of the IFLG in presence of gravity [18], showing that at low Γ the system is frozen in a SG-like phase, but at higher Γ it separates in a frozen SG phase at the bottom and a fluid phase on top. Above a critical Γ the system is entirely fluid [19].

A. “Irreversible-reversible” cycles and the dynamical glass transition

Tapping experiments typically show “irreversible-reversible” cycles [4] (see Fig.3): during a sequence of taps, if the system is successively shaken at increasing vibration amplitudes,

its bulk density typically grows, as in compaction, and then, after a characteristic Γ_{ex} starts decreasing. However, if the amplitude of shaking is decreased back to zero, the density generally doesn't follow the same path since it keeps growing. In this sense these observations outlines the existence of “memory effects”.

In analogy to real experiments, cycles of taps were performed in the IFLG in which the vibration amplitude Γ was varied in sequences of increments $\gamma = \Delta\Gamma/\tau$, with constant taps duration τ . After each tap the static bulk density of the system $\rho(\Gamma_n)$ (n is the n -th tap number) was then measured. The data are qualitatively very similar to those reported in real experiments on dry granular packs [4]. Furthermore, they allow to define a “jamming” transition point $\Gamma_g(\gamma)$ in analogy to the glass transition in glass formers [13], as explained in Fig.4.

B. Two-times correlation functions

Granular media in the above dynamical situations show “aging” too [13]. To see this, as much as in glassy systems, it is useful to consider two time correlation functions as ($t \geq t'$): $C(t, t') = [\langle \rho(t)\rho(t') \rangle - \langle \rho(t) \rangle \langle \rho(t') \rangle] / [\langle \rho(t')^2 \rangle - \langle \rho(t') \rangle^2]$ where $\rho(t)$ is the bulk density of the system at time t .

The fit, at low Γ , of the two time correlation function, $C(t, t')$, (on five decades in MC time), reveals the following interesting approximate scaling form:

$$C(t, t') = (1 - c_\infty) \frac{\ln[(t' + t_s)/\tau]}{\ln[(t + t_s)/\tau]} + c_\infty \quad (4)$$

where τ (which now is not the “tap duration” as before), t_s and c_∞ are fit parameters. Very interesting is the fact that the above behaviour is found in both the discussed models (Tetris and IFLG) [13]. The data for the two models, for several values of Γ , rescaled on a single universal master function, are plotted in Fig. 5. It is interesting the existence of such a scaling behaviours in off equilibrium dynamics of apparently different systems [24].

C. Response functions and the “fluctuation-dissipation” relation

In Ref. [14] it was argued that in granular media it is possible to formulate a link between response and fluctuations, i.e., the analogous of a “fluctuation dissipation theorem” (FDT) (see [20]), where the amplitude of external vibrations plays the role of the usual “temperature”. In typical situations the FDT coincides neither with its usual version at equilibrium nor with the extensions valid in off equilibrium thermal systems in the so called “small entropy production” limit [21]. The origin of universalities in off equilibrium dynamics in the above heterogeneous classes of materials is still unanswered.

Our systems are “shaken” at a given amplitude x_0 and the average grains height, $h_0(t) = \langle H(t) \rangle$ (with $H(t) = \sum_i y_i(t)/N$), recorded as long as the “mean square displacement” $B(t, t') \equiv \langle [H(t) - H(t')]^2 \rangle$. To measure the response function, the average height, $h_1(t, t_w)$, was also recorded in an identical copy of the system (a “replica”) perturbed by a small increase of the shaking amplitude, after a time t_w .

The difference in heights between the perturbed and unperturbed systems $\Delta h(t, t_w) = h_1(t, t_w) - h_0(t)$ is by definition the integrated response. FDT or its generalisations concern the relation between $\Delta h(t, t_w)$ and the displacement, $B(t, t_w)$. In analogy to thermal systems [9], in Ref. [14] was proposed that:

$$\Delta h(t, t_w) \simeq \frac{X}{2} \Delta(\Gamma^{-1}) B(t, t_w) \quad (5)$$

Eq.(5) states that, after transients, in a granular system the measure of the height variation after a change in shaking amplitude, should be proportional to the “displacement” recorded during an unperturbed run. In the simplest situations, as equilibrium thermal systems, the proportionality factor, X , is a constant, but more generally, X is function of t_w and t themselves. Interestingly, in glassy systems the quantity $g\Gamma/X$ has the meaning of an “effective temperature” [22,23].

In the present model, eq. (5) seems to be approximately valid, also if in typical off-equilibrium situations X slowly depends on Γ and t_w . This is shown, for high x_0 , in the

top panels of Fig.6: in the long time regime X is equal to 1, showing that, in the high “temperature” and low density region, the usual equilibrium version of FDT is obeyed. In the low x_0 region, the above picture changes, as shown in the bottom panels Fig.6: after an early transient the response, Δh , is *negative* and, thus, X is negative, which would asymptotically correspond to a negative “effective temperature”.

V. CONCLUSIONS

In conclusion, the present paper has dealt with the understanding of the “jamming” transition in granular media via the introduction of models from standard statistical mechanics to describe these “non-thermal” systems (the IFLG and Tetris, [6,7]).

They exhibit a logarithmic compaction when subject to gentle shaking in presence of gravity, a compaction extremely close to what is experimentally observed in granular packs [3]. The presence of such slow dynamics is linked to the existence of a “jamming” transition in granular media. In fact, in the high density region, at ρ_m , the models undergo a structural arrest where grains self-diffusivity becomes zero [6].

Self-diffusion suppression at ρ_m signals that, above such a density, it is impossible to obtain a macroscopic rearrangement of grains without increasing the system volume, a fact interestingly similar to the phenomenon of the Reynolds dilatancy transition [6].

A very important fact is that results from the present models are in excellent agreement with known experimental ones, and their many new outcomes must be still experimentally investigated. We have also discussed the intriguing connections of granular media with others materials, as glassy systems or spin glasses, where geometrical disorder and frustration play a crucial role.

VI. ACKNOWLEDGEMENTS

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FIGURES

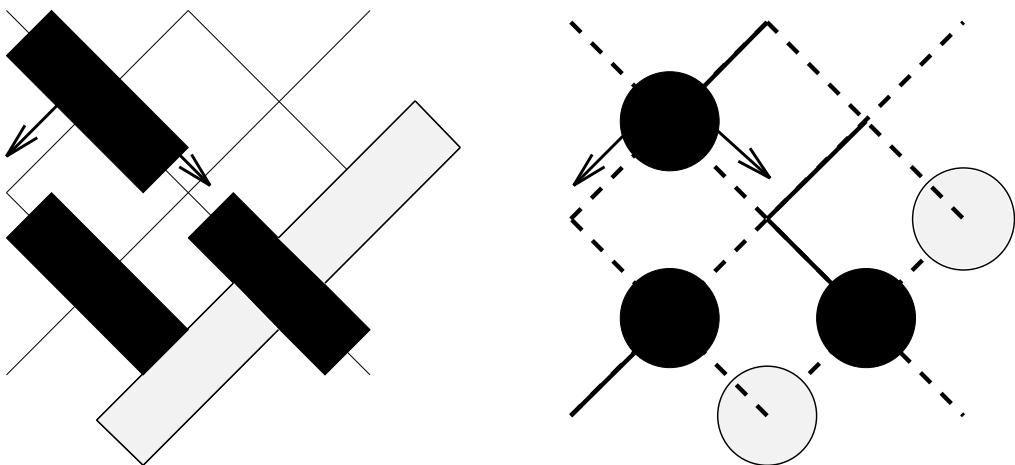


FIG. 1. A schematic picture of the two kind of frustrated lattice gas models described in the text. *Left:* the Tetris model. *Right:* the Ising Frustrated Lattice Gas, IFLG. Straight and dashed lines represent the two kind of interactions $\epsilon_{ij} = \pm 1$. Filled circles are present particles with “orientation” $S_i = \pm 1$ (black/white).

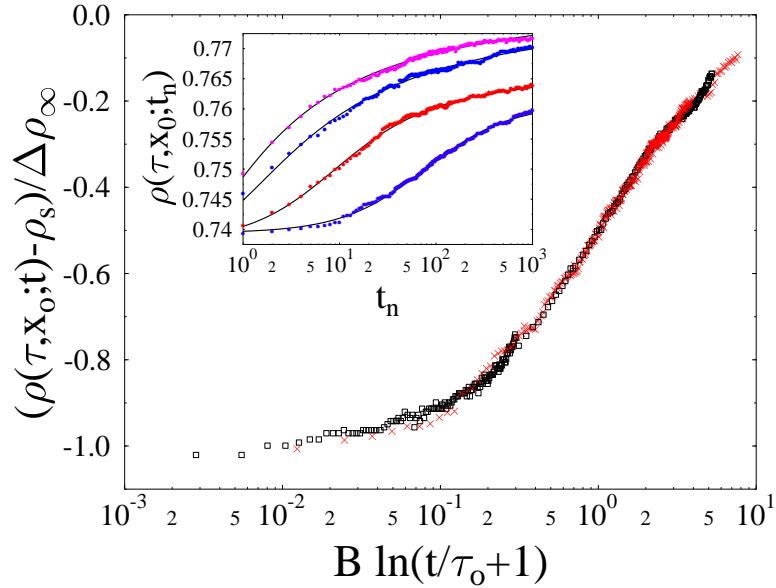


FIG. 2. The compaction of granular media at low shaking amplitudes. Experimental data from Knight et al. (squares) and MC data about IFLG (circles) rescaled according eq. (3). Insert: density $\rho(\tau, x_0; t_n)$ from MC data as a function of tap number t_n , for tap amplitudes $x_0 = 0.001, 0.01, 0.05, 0.1$ (from bottom to top) and duration $\tau = 3.28 \cdot 10^1$. The superimposed curves are logarithmic fits from eq. (3).

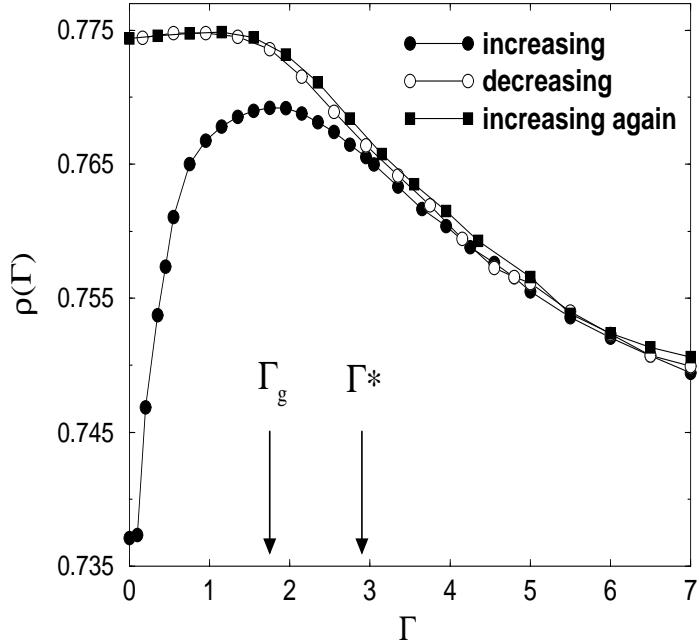


FIG. 3. The static bulk density, $\rho(\Gamma)$, of the IFLG model as a function of the vibration amplitude, Γ , in cyclic vibration sequences. The system is shaken with an amplitude Γ which at first is increased (filled circles), then is decreased (empty circles) and, finally, increased again (filled squares) with a given “annealing-cooling” velocity $\gamma \equiv \Delta\Gamma/\tau$. Here we fixed $\gamma = 1.25 \cdot 10^{-3}$. The upper part of the cycle is approximately “reversible” (i.e., empty circles and filled squares fall roughly on the same curve). The data compare rather well with the experimental data of Novak et al.. Γ^* is approximately the point where the “irreversible” and the “reversible” branches meet. Γ_g signals the location of a “jamming transition”.

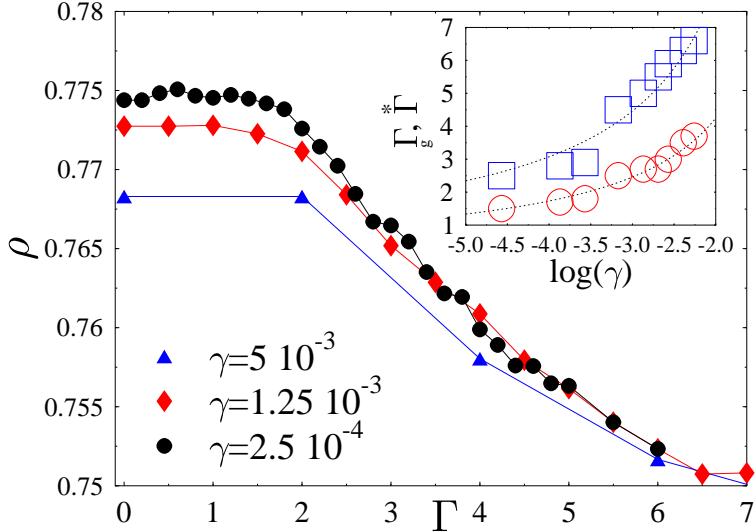


FIG. 4. *Main frame:* As in Fig.3, the density, $\rho(\Gamma)$, is plotted as a function of the vibration amplitude, Γ for three values of the “cooling” velocity γ . Here only the descending parts of the cycles are shown. As in glasses, a too fast cooling drives the system out of equilibrium. The position of the shoulder, $\Gamma_g(\gamma)$, schematically individuates a “jamming transition”. *Inset:* numerical estimate, in the IFLG model of the dependence of $\Gamma_g(\gamma)$ (circles) and $\Gamma^*(\gamma)$ (squares) on the cooling rate γ . Superimposed are logarithmic fits in analogy to those for the glass transition temperature, $T_g(\gamma)$, in glasses [4]. When $\gamma \rightarrow 0$ we roughly find $\Gamma_g(0) = \Gamma^*(0)$.

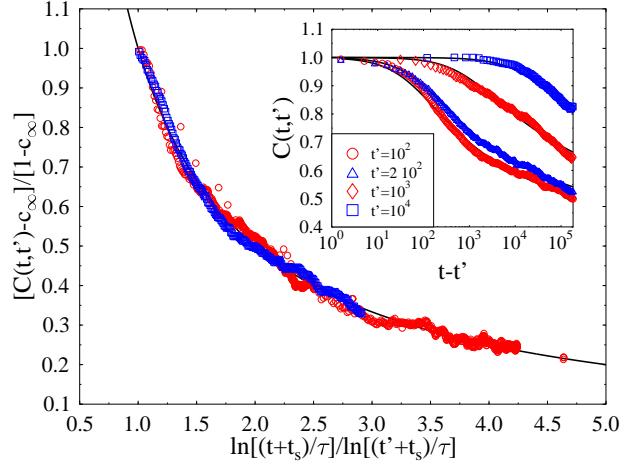


FIG. 5. The two time density-density correlation function, $(C(t, t') - c_\infty)/(1 - c_\infty)$, as a function of the scaling variable $\alpha = \ln[(t + t_s)/\tau]/\ln[(t' + t_s)/\tau]$. Scaled on the same master function are data from both models considered in the present paper (Tetris, squares, and IFLG, circles) for $\Gamma = -1/\ln(x_0)$ with $x_0 \in [10^{-4}, 10^{-1}]$. *Inset:* The correlation $C(t, t')$ for the Tetris at $\Gamma = 0.22$ (or $x_0 = 0.01$) as a function of $t - t'$ for $t' = 10^2, 2 \cdot 10^2, 10^3, 10^4$.

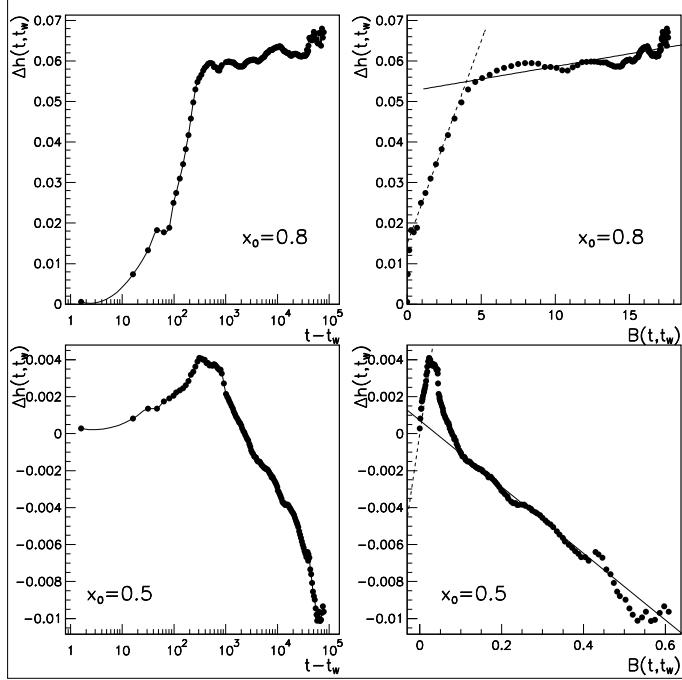


FIG. 6. The figures on the left show, as a function of $t - t_w$, the average height difference, $\Delta h(t, t_w) \equiv h_1(t, t_w) - h_0(t)$, of a reference system shaken at a given x_0 and a replica perturbed after t_w by shaking at $x_0 + \Delta x_0$ ($\Delta x_0 = .002$). On the right, a check of the generalized fluctuation dissipation relation of eq. (5) is given. The integrated response, $\Delta h(t, t_w)$, is plotted as a function of the displacement of the reference system, $B(t, t_w)$. Systems are shaken at different “amplitudes” x_0 ($x_0 = 0.8$ top, $x_0 = 0.5$ bottom), with replicas perturbed after a $t_w = 370$. At low x_0 , negative responses appear, but in agreement with eq. (5), Δh is asymptotically still approximately linear in B .